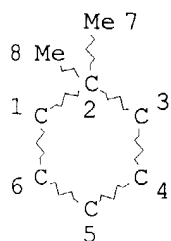


=> d que 141

L12 STR

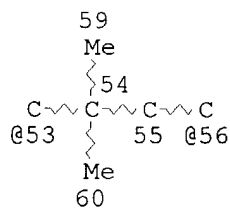
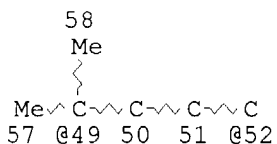
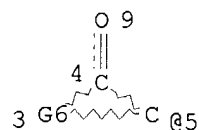
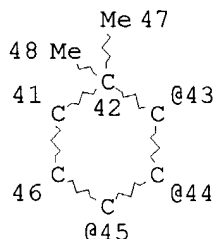
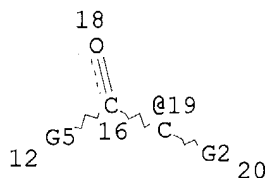


NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 2
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
 L16 STR

G1=G4 CH\Ak
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VAR G1=5/19
 VAR G2=H/ME
 VAR G4=CH2/39
 VAR G5=43/44/45
 VAR G6=49-4 52-5/52-4 49-5/53-4 56-5/56-4 53-5

NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE

L18 7978541 SEA FILE=REGISTRY ABB=ON PLU=ON C6/ES AND O/ELS AND NC=1 NOT
(PMS OR IDS)/CI AND NR<5 AND C>10
L20 398 SEA FILE=REGISTRY SUB=L18 SSS FUL L12 AND L16
L21 317 SEA FILE=HCAPLUS ABB=ON PLU=ON L20(L)PREP/RL
L28 TRANSFER PLU=ON L21 1- RN : 5326 TERMS
L29 5326 SEA FILE=REGISTRY ABB=ON PLU=ON L28
L30 STR

~~O=C-C~~
1 2 3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L32 3515 SEA FILE=REGISTRY SUB=L29 SSS FUL L30
L33 STR

CH=O
1 2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE

L35 264 SEA FILE=REGISTRY SUB=L29 SSS FUL L33
L36 280202 SEA FILE=HCAPLUS ABB=ON PLU=ON L32(L) (RACT OR RCT OR RGT)/RL
L37 114368 SEA FILE=HCAPLUS ABB=ON PLU=ON L35(L) (RACT OR RCT OR RGT)/RL
L38 98133 SEA FILE=HCAPLUS ABB=ON PLU=ON L36 AND L37
L39 111 SEA FILE=HCAPLUS ABB=ON PLU=ON L38 AND L21
L40 4 SEA FILE=REGISTRY ABB=ON PLU=ON L29 AND (TI OR ZR OR HF)/ELS
L41 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND L40

=> d l41 ibib abs hitind hitstr

L41 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:906114 HCAPLUS
DOCUMENT NUMBER: 138:4201
TITLE: Catalytic system for aldol reactions
INVENTOR(S): Jacoby, Denis
PATENT ASSIGNEE(S): Firmenich Sa, Switz.
SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002094755	A1	20021128	WO 2002-IB1839	20020521
W: CN, IL, IN, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1395542	A1	20040310	EP 2002-730616	20020521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2004082818	A1	20040429	US 2003-688297	20031017
PRIORITY APPLN. INFO.:				
			WO 2001-IB902	W 20010522
			WO 2002-IB1839	W 20020521

OTHER SOURCE(S): CASREACT 138:4201; MARPAT 138:4201

AB The invention relates to a process for the preparation, in a single step, of enones by an aldol condensation of a ketone, such as a gem-dimethylcyclohexylethanone or gem-dimethylcyclohexenylethanone derivative, with an aldehyde in the presence of a novel catalytic system and without the pre-formation of an enolate. Said catalytic system consists of a metal complex, such as a [(Cl)_n(alkoxy)_{4-n}Ti] or [(Cl)_n(alkoxy)_{4-n}Zr] complex (n = 1-3), and a co-ingredient, such as a carboxylic acid anhydride or an anhydrous salt. Thus, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-1-ethanone was treated with MeCHO in presence of Zr(OPr)Cl₃ and MgCl₂ to give 45% 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one.

IC ICM C07C045-72

ICS C07C049-557; B01J031-12

CC 21-2 (General Organic Chemistry)

IT 106-31-0, Butyric anhydride 108-24-7, Acetic anhydride 123-62-6, Propionic anhydride 3981-83-7, Isopropoxytitanium trichloride 7637-07-2, Boron trifluoride, uses 7705-08-0, Iron(III) chloride, uses 7757-82-6, Sodium sulfate, uses 7778-80-5, Potassium sulfate, uses 7786-30-3, Magnesium chloride, uses 31676-28-5, Dipropoxyzirconium dichloride 113133-11-2
 RL: CAT (Catalyst use); USES (Uses)
 (catalytic system for aldol reactions)

IT 71048-82-3P

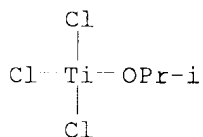
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
 (catalytic system for aldol reactions)

IT 50-00-0, Formaldehyde, reactions 75-07-0, Acetaldehyde, reactions 78-93-3, 2-Butanone, reactions 107-02-8, 2-Propenal, reactions 830-13-7, Cyclododecanone 1193-47-1, 2,2-Dimethylcyclohexanone 1197-92-8 4170-30-3, 2-Butenal 37709-66-3 41435-93-2 41436-46-8 54201-08-0 55981-43-6 73956-68-0 91819-58-8 476689-60-8 476689-61-9 476689-64-2 476689-65-3

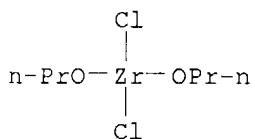
RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalytic system for aldol reactions)

IT 565-62-8P 23696-85-7P 57020-37-8P 65113-95-3P 83218-16-0P 255058-92-5P 344296-64-6P 476689-62-0P 476689-63-1P

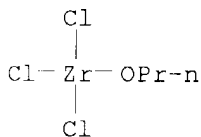
RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (catalytic system for aldol reactions)
 IT **3981-83-7**, Isopropoxytitanium trichloride **31676-28-5**,
 Dipropoxyzirconium dichloride **113133-11-2**
 RL: CAT (Catalyst use); USES (Uses)
 (catalytic system for aldol reactions)
 RN 3981-83-7 HCAPLUS
 CN Titanium, trichloro(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



RN 31676-28-5 HCAPLUS
 CN Zirconium, dichlorodipropoxy-, (T-4)- (9CI) (CA INDEX NAME)

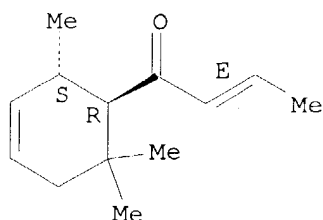


RN 113133-11-2 HCAPLUS
 CN Zirconium, trichloropropoxy-, (T-4)- (9CI) (CA INDEX NAME)

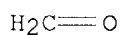


IT **71048-82-3P**
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**
(Preparation)
 (catalytic system for aldol reactions)
 RN 71048-82-3 HCAPLUS
 CN 2-Buten-1-one, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, (2E)-rel-
 (9CI) (CA INDEX NAME)

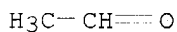
Relative stereochemistry.
 Double bond geometry as shown.



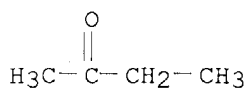
IT 50-00-0, Formaldehyde, reactions 75-07-0, Acetaldehyde,
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 2-Propenal, reactions 830-13-7, Cyclododecanone
 1193-47-1, 2,2-Dimethylcyclohexanone 1197-92-8
 4170-30-3, 2-Butenal 37709-66-3 41435-93-2
 41436-46-8 54201-08-0 55981-43-6
 73956-68-0 91819-58-8 476689-60-8
 476689-61-9 476689-64-2 476689-65-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalytic system for aldol reactions)
 RN 50-00-0 HCAPLUS
 CN Formaldehyde (8CI, 9CI) (CA INDEX NAME)



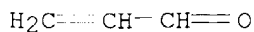
RN 75-07-0 HCAPLUS
 CN Acetaldehyde (8CI, 9CI) (CA INDEX NAME)



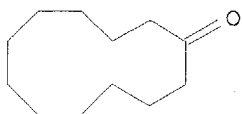
RN 78-93-3 HCAPLUS
 CN 2-Butanone (8CI, 9CI) (CA INDEX NAME)



RN 107-02-8 HCAPLUS
 CN 2-Propenal (9CI) (CA INDEX NAME)

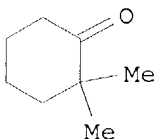


RN 830-13-7 HCAPLUS
 CN Cyclododecanone (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



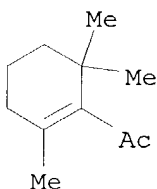
RN 1193-47-1 HCAPLUS

CN Cyclohexanone, 2,2-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



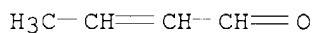
RN 1197-92-8 HCAPLUS

CN Ethanone, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



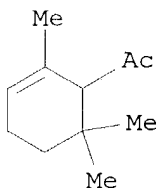
RN 4170-30-3 HCAPLUS

CN 2-Butenal (9CI) (CA INDEX NAME)



RN 37709-66-3 HCAPLUS

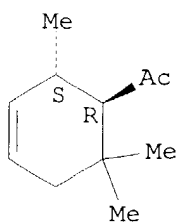
CN Ethanone, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



RN 41435-93-2 HCAPLUS

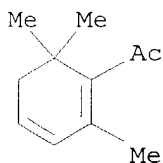
CN Ethanone, 1-[(1R,2S)-2,6,6-trimethyl-3-cyclohexen-1-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



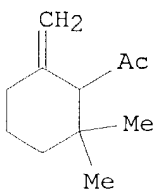
RN 41436-46-8 HCAPLUS

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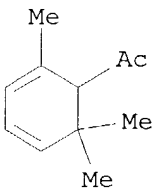
RN 54201-08-0 HCAPLUS

CN Ethanone, 1-(2,2-dimethyl-6-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



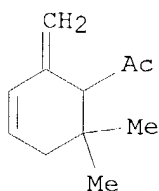
RN 55981-43-6 HCAPLUS

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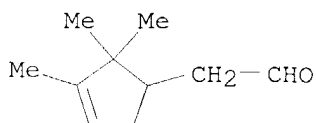
RN 73956-68-0 HCAPLUS

CN Ethanone, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



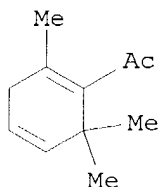
RN 91819-58-8 HCAPLUS

CN 3-Cyclopentene-1-acetaldehyde, 2,2,3-trimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



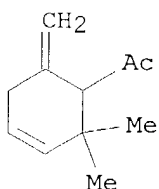
RN 476689-60-8 HCAPLUS

CN Ethanone, 1-(2,6,6-trimethyl-1,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



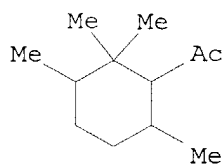
RN 476689-61-9 HCAPLUS

CN Ethanone, 1-(2,2-dimethyl-6-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)

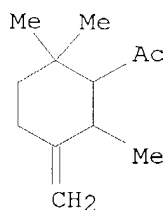


RN 476689-64-2 HCAPLUS

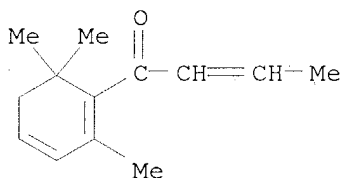
CN Ethanone, 1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



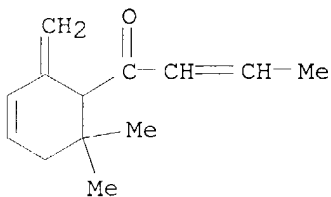
RN 476689-65-3 HCAPLUS
 CN Ethanone, 1-(2,2,6-trimethyl-5-methylenecyclohexyl)- (9CI) (CA INDEX NAME)



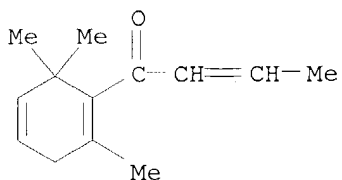
IT 23696-85-7P 57020-37-8P 83218-16-0P
 255058-92-5P 476689-62-0P
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (catalytic system for aldol reactions)
 RN 23696-85-7 HCAPLUS
 CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)- (8CI, 9CI) (CA INDEX NAME)



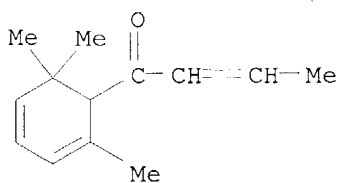
RN 57020-37-8 HCAPLUS
 CN 2-Buten-1-one, 1-(6,6-dimethyl-2-methylene-3-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



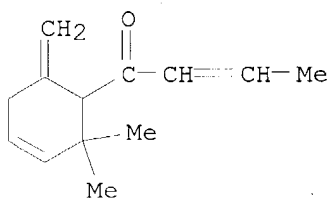
RN 83218-16-0 HCAPLUS
 CN 2-Buten-1-one, 1-(2,6,6-trimethyl-1,4-cyclohexadien-1-yl)- (9CI) (CA INDEX NAME)



RN 255058-92-5 HCAPLUS

CN 2-Buten-1-one, 1-(2,6,6-trimethyl-2,4-cyclohexadien-1-yl)- (9CI) (CA
INDEX NAME)

RN 476689-62-0 HCAPLUS

CN 2-Buten-1-one, 1-(2,2-dimethyl-6-methylene-3-cyclohexen-1-yl)- (9CI) (CA
INDEX NAME)

REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT